



**>>Entry Name: Diisopropyl sulfide**

**Synonym(s):** 2,2'-Thiobispropane, 9Cl. Isopropyl sulfide, 8Cl

**CAS Registry Number:** 625-80-9

$(\text{H}_3\text{C})_2\text{CHSCH}(\text{CH}_3)_2$

**Molecular Formula:**  $\text{C}_6\text{H}_{14}\text{S}$

**Molecular Weight:** 118.243

**Accurate Mass:** 118.08162

**Percentage Composition:** C 60.95%; H 11.93%; S 27.12%

**Boiling Point:** Bp 120-121°

**Density:**  $d_4^{20}$  0.814

**Refractive Index:**  $n_D^{20}$  1.4381

**Aldrich:** I-2680-9

**>>Derivative: S-Oxide**

**Synonym(s):** 2,2'-Sulfinylbispropane, 9Cl. Diisopropyl sulfoxide

**CAS Registry Number:** 2211-89-4

**Molecular Formula:**  $\text{C}_6\text{H}_{14}\text{OS}$

**Molecular Weight:** 134.242

**Accurate Mass:** 134.076535

**Percentage Composition:** C 53.68%; H 10.51%; O 11.92%; S 23.89%

**Boiling Point:** Bp<sub>0.9</sub> 59°

**>>Derivative: S,S-Dioxide**

**Synonym(s):** 2,2'-Sulfonylbispropane, 9Cl. Diisopropyl sulfone

**CAS Registry Number:** 595-50-6

**Molecular Formula:**  $\text{C}_6\text{H}_{14}\text{O}_2\text{S}$

**Molecular Weight:** 150.241

**Accurate Mass:** 150.07145

**Percentage Composition:** C 47.97%; H 9.39%; O 21.30%; S 21.34%

**Physical Description:** Cryst. ( $\text{Et}_2\text{O}$ )

**Melting Point:** Mp 36°

**Boiling Point:** Bp<sub>0.5</sub> 78°

**Solubility:** Sol.  $\text{H}_2\text{O}$

**Rare Chemicals Library:** S79909-2

**References:**

*Aldrich Library of  $^{13}\text{C}$  and  $^1\text{H}$  FT NMR Spectra*, 1992, **1**, 430B, (*nmr*)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 267D, (*ir*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 351C, (*ir*)

Claus, A., *Ber.*, 1875, **8**, 532, (*synth*)

Cumper, C.W.N. *et al.*, *J.C.S.(A)*, 1966, 239; 323, (*synth, uv*)